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A PIECEWISE LINEAR DISCONTINUOUS FINITE ELEMENT SPATIAL DISCRETIZATION OF THE S_N TRANSPORT EQUATION FOR POLYHEDRAL GRIDS IN 3D CARTESIAN GEOMETRY

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Introduction

We introduce a new spatial discretization of the linear Boltzmann transport equation for 3D Cartesian geometry. This spatial discretization, called the Piecewise Linear Discontinuous Finite Element method (PWLD), is a standard Galerkin DFEM method that utilizes Piecewise Linear basis functions, which were first used in 2D by Stone and Adams[1,2], and in 3D for a CFEM diffusion discretization[3]. The PWLD method is designed for accuracy in the thick diffusion limit on arbitrary polyhedral grids. Previously, only Corner Balance methods have been shown to be successful in the diffusion limit for these 3D grid types [4,5]. Other methods that may be extended to 3D for polyhedral grids include DFEMs using Wachspress basis functions [6,7], the CFEM-based DFEM methods developed by Warsa [8], and characteristics methods that use PWL source approximations [9]. We will briefly derive the PWLD method for polyhedral grids and present a variety of numerical methods to demonstrate its numerical resiliency and correctness. Furthermore, we note that the PWLD method meets all of Adams' requirements for acceptable diffusion limit behavior [10] on polyhedral grids, but will not show numerical results to this effect. The goal of this paper is to serve as an introduction to the application of PWLD for 3D transport.

Development

We write the time-independent, monoenergetic Sn transport equation in 3D Cartesian geometry as

$$\vec{\Omega}_m \bullet \vec{\nabla} \psi_m(x,y,z) + \sigma(x,y,z)\psi_m(x,y,z) = Q_m(x,y,z), \qquad (1)$$

where the *m* subscript indicates the index of an element in the quadrature set used for the discrete-ordinates approximation [11].

The application of a DFEM to this equation is straightforward, and described in many different references [1,2,6,8,10,12,13]. DFEMs expand all spatially dependent terms (ψ and Q in Eq. (1)) in terms of basis functions, u. For convenience when working with polyhedral cells, we divide our cells into tetrahedral sub-cell units, called sides. We define a side by two adjacent vertices, a face center point, and the cell center point. Because a face can be determined by more than three vertices, the vertices on a face do not have to be co-planar in general. As a result, we facet our face about the face center point. A side for a faceted face is shown in Figure 1.

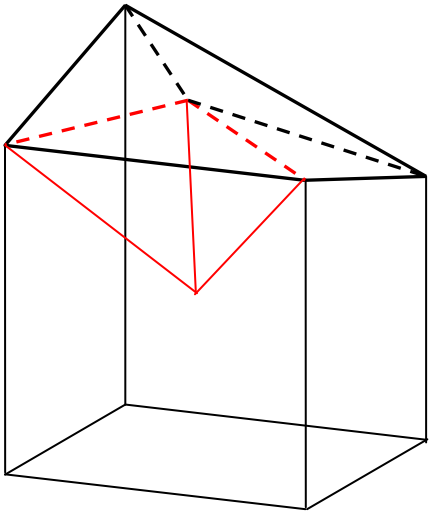

Figure 1: A side in a hexahedral cell with a faceted face

We now define the basis functions as linear combinations of the standard linear functions on tetrahedral sides:

$$u_j(\vec{r}) \;=\; t_j(\vec{r}) \;+\; \sum_{faces\ at\ j} \beta_{f,j} t_f(\vec{r}) \;+\; \alpha_{c,j} t_c(\vec{r}), \tag{2}$$

where the t functions are standard linear functions defined tetrahedron by tetrahedron. For example, t_j equals one at the j-th vertex and decreases linearly to zero on all other vertices of each side that touches point j. t_c is unity at the cell midpoint and zero at each face midpoint and each cell vertex. t_f is unity at the face midpoint and zero at the cell midpoint and at each of the face's vertices. The α_c and β_f are weights that give the cell and face midpoints as weighted averages of their vertices:

$$\vec{r}_c \equiv \text{ cell midpoint} = \sum_{j@c} \alpha_{c,j} \vec{r}_j \;; \tag{3}$$

$$\vec{r}_f \equiv \text{ face midpoint} = \sum_{j@f} \beta_{f,j} \vec{r}_j \,. \tag{4}$$

In this paper we assume that $\alpha_{c,j} = \frac{1}{J}$ and $\beta_{f,j} = \frac{1}{N_f}$, where *J* is the number of vertices in the cell, and N_f is the number of vertices in a face. As a result, α is the same for every basis function in the cell, and β_f is the same for every basis function on a face. We note that this basis function definition meets Adams' diffusion limit requirement of full-resolution for DFEMs [10] because we can define a basis function supported at each node in a general polyhedral cell.

The result of the DFEM discretization is a single-cell matrix that determines the unknowns in each cell in terms of its source and its incident intensities (from upstream cells or boundary conditions). The size of the single cell matrix is *JxJ* where *J* is the number of basis functions used to approximate the flux in the cell. A row of a single-cell matrix is determined by testing the equation with a weight function. The ith row of the single cell matrix is given by

$$\begin{aligned}
&\sum_{\substack{f=face\\ @i}} \sum_{s \in f} \left(\vec{\Omega}_m \bullet \vec{n}\right)_s \int_{\partial V_s} v_i \left[\left(\sum_{j=1}^{J} \tilde{\psi}_{m,f,j} u_j(x,y,z) \right) - \left(\sum_{j=1}^{J} \psi_{m,j} u_j(x,y,z) \right) \right] ds \\
&\qquad + \sum_{s \in cell} \int_{V_s} v_i \left[\vec{\Omega}_m \bullet \vec{\nabla} \left(\sum_{j=1}^{J} \psi_{m,j} u_j(x,y,z) \right) \right] dV \\
&+ \sum_{s \in cell} \int_{V_s} v_i \left[\sigma(x,y,z) \sum_{j=1}^{J} \psi_{m,j} u_j(x,y,z) \right] dV = \sum_{s \in cell} \int_{V_s} v_i \sum_{j=1}^{J} Q_{m,j} u_j(x,y,z) dV
\end{aligned} \tag{5}$$

where $\tilde{\psi}_m$ denotes an angular intensity unknown on the boundary of the cell. These surface quantities are determined by an upwinding condition.

$$\tilde{\psi}_m = \begin{cases} \psi_{m,cell} \;\; if \;\; \vec{n} \bullet \vec{\Omega}_m > 0 \\ \psi_{m,upwind\ cell} \;\; if \;\; \vec{n} \bullet \vec{\Omega}_m < 0 \end{cases}. \tag{6}$$

The upwinding condition along with the weight and basis function definitions allows this method to retain the surface matching property requirement for the diffusion limit [10]. Again, for convenience when working with polyhedral cells, the integrals in Eq. (5) are divided into sums of integrals over sides. Eqs. (5) and (6) represent a general discontinuous finite element spatial discretization applied to the 3D Cartesian transport equation. We solve the system of equations local to a cell

generated by multiplying Eq. (5) by J distinct weight functions $\{v_i\}$, which are the same set of equations as the basis functions, to produce an approximate solution to the transport equation in the cell. We have now fully defined our method except for boundary conditions, which are straightforward. We have also developed a lumped and lumping parameter version of the method, which we will not describe in detail in this paper [12].

Numerical Test Problems

We have developed a variety of numerical test problems to further characterize our method and compare it against existing methods. We implemented our method in the Parallel Deterministic Transport Code (PDT) being developed at Texas A&M University. PDT is a massively parallel code that is designed to be a general methods test bed for deterministic transport. We have also implemented unlumped, lumped, and lumping parameter versions of the Tri-Linear DFEM (TriLD) [13] in PDT, and use it as a standard by which to compare the accuracy of PWLD.

The first test problem we will present tests the resiliency of the method on extremely distorted cells. In this test problem, we have a one cell spatial domain of 4 cm x 4 cm x 4 cm, ranging from the point (0,0,0) to the point (4,4,4). The vertex at the origin, (0,0,0), is moved incrementally toward the vertex located at (4,4,4). That is, we begin with a cube and incrementally make it closer to concave, slightly concave, and ultimately dramatically concave. As we do this, some of the faces become significantly non-planar. Moreover, some of the "side" subcells take on negative volumes when the cell center point is outside the cell, which is true for some of tests.

The next set of test problems are truncation error test problems. We ran a series of truncation error problems in the thin limit, and compared the results of PWLD and TriLD. For these truncation error problems we developed a problem with a quadratic solution using the method of manufactured solutions [12]. These quadratic solutions have spatial coordinate cross-terms which are contained in the TriLD solution space, but not in the PWLD solution space. As a result, TriLD has an advantage for this test problem. We will show that all methods produce a second-order truncation error rate and very similar accuracy.

Finally, we will present PDT solutions to a selected set of the Kobayashi 3-D Radiation Transport Benchmark problems[14]. We will also make some comments about PDT computational performance on these and other problems.

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